

# CHEMISTRY AND MATERIALS SCIENCE DIRECTORATE NEWS

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs

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## Message from the Associate Director

As I look back at the past fiscal year (FY)—my first as associate director (AD) of the Chemistry and Materials Science (CMS) Directorate—I'd like to reflect on the year's accomplishments, both in CMS and at the Laboratory.

When I accepted the AD assignment, I talked to all of you about the need for balance and excellence in all our endeavors, and we discussed how to take our directorate to the next level.

It was important then—just as it is now—to meet our commitments to various Laboratory programs: Defense and Nuclear Technologies (DNT); National Ignition Facility (NIF) Programs; Nonproliferation, Arms Control, and International Security (NAI); Homeland Security; and Energy & Environment (E&E).

I placed a similar emphasis on continuing our excellence in science to enable the future Laboratory mission.

[Continued on page 10 >](#)

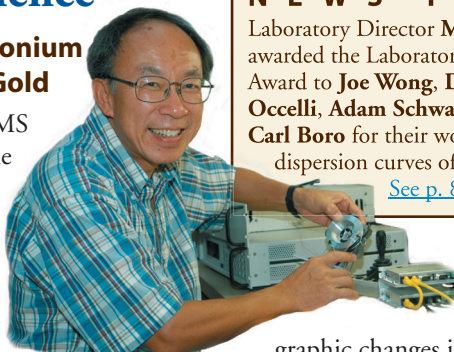
chemistry &  
materials  
science  
**CMS**

## Corner on Science

### Joe Wong's First Plutonium Experiment Strikes Gold

About 18 months ago, CMS scientist **Joe Wong** became curious about plutonium (Pu) science. He had never conducted any Pu research and wanted to see what new experiments could be done. After reading *Challenges in Plutonium Science*, Joe discovered that many articles in the two-volume compilation mentioned the importance of phonon dispersion curves (PDCs), yet no data had ever been collected on Pu PDCs.

Phonons, or lattice vibrations, are the acoustic equivalent of photons (the basic quanta of light). PDCs describe how atoms move within a solid and determine many physical properties, such as sound velocity, elasticity, and phase stability. These properties are highly anomalous in Pu, making the understanding of phonons key. The mechanisms behind Pu's phase stability are especially important because



CMS scientist Joe Wong with the sample holder used in his plutonium experiments.

## NEWS FLASH

Laboratory Director **Michael Anastasio** has awarded the Laboratory's Science and Technology Award to **Joe Wong, Dan Farber, Florent Ocelli, Adam Schwartz, Mark Wall, and Carl Boro** for their work measuring the phonon dispersion curves of  $\delta$ -plutonium-gallium.

[See p. 8 for more information.](#)

Pu exists in many phases, undergoing crystallographic changes involving phonons during each phase transformation.

Joe learned that despite 40 years of attempts, two main obstacles had prevented the experimental determination of Pu PDCs. First, inelastic neutron scattering (INS), the leading method for determining PDCs, requires single-crystal samples measuring at least 1 cm<sup>3</sup>. However, Pu has repeatedly defied attempts to grow such crystals. Even if large Pu crystals were available, they would have to be made from a rare Pu isotope, <sup>242</sup>Pu, because the other Pu isotopes tend to absorb neutrons, thus stripping INS of its power.

To counter these obstacles, Joe considered a recently developed microbeam

[Continued on page 8 >](#)

## Interview With...

### Kim Budil

In June 2003, **Kim Budil** left the Defense and Nuclear Technologies (DNT) Directorate and joined CMS. As the new associate division leader for dynamic experiments in the Materials Science and Technology Division (MSTD), Kim is helping to develop a program to study

the properties and performance of materials under extreme conditions. Her vision is



to promote and expand the computational and experimental expertise in MSTD so that the division is recognized as the world leader in dynamic materials research.

Kim is also the manager of Campaign 2 (Dynamic Materials Properties) at the Department of Energy (DOE) headquarters in Washington, D.C. In this two-year assignment, Kim coordinates the various elements of Campaign 2 at Livermore, Los Alamos, Sandia, and other university and DOE laboratory participants, while also gaining an overview of the Defense Programs enterprise and using her technical expertise to help DOE headquarters understand the wealth of resources available through the national laboratories.

[Continued on page 9 >](#)

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## Directorate News

### CMS Technology Featured on the History Channel

**Randy Simpson**, the division leader  
of the Chemistry and Chemical  
Engineering Division, recently  
appeared on a History Channel pro-  
gram titled "Terror Tech: Defending  
the Highrise." The episode, which  
aired on August 12 as part of the  
History Channel's *Modern Marvels*  
series, featured new technologies that  
are being developed to counter terrorism.

As one of several Livermore scien-  
tists who appeared on the show, Randy  
discussed the work of the Energetic  
Materials Center in creating high-  
explosives simulants—nonexplosive  
materials that exhibit the same char-  
acteristics (appearance, smell, etc.) as  
actual explosives. Such simulants, or

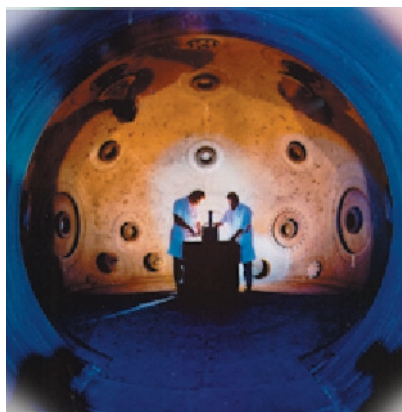


The  
Laboratory's High  
Explosives Application Facility (HEAF).

"bogus bombs," can be used to train  
bomb-sniffing dogs and to calibrate  
explosives-detection equipment without  
fear of accidental explosion. The episode  
also included footage of high-explosives  
experiments conducted in the 10-kg  
spherical chamber at the Laboratory's  
High Explosives Application Facility.

Randy will also appear in an  
upcoming episode of *Tactical to Practical*,  
a new History Channel series that  
highlights the evolution of innovations  
developed for combat into useful tools  
for civilian life. For this series, Randy  
again discussed CMS's work with  
energetic materials, which fit well with  
the episode's focus on the intertwined  
industrial and military applications of  
energetic materials—rocket propellants,  
explosives, and pyrotechnics—dating  
back to the invention of gunpowder.

CMS applauds the continued  
excellence of the Energetic Materials  
Center and thanks Randy for explain-  
ing our national-security efforts to the  
outside community. ■



The HEAF's 10-kg spherical chamber, where many  
CMS experiments involving high explosives are  
performed.

### CMS Information Management Is Now Fully Electronic

In September, CMS became the second  
directorate to begin using the new, fully  
electronic information management  
(IM) system, which replaces the  
Laboratory's previous review  
and release process. The  
new system allows authors  
to track the status of their  
document reviews online,  
use electronic signatures, and  
upload their final documents to  
the IM Web site for automatic conver-  
sion to PDFs.

To start a new document review,  
simply visit <http://im.llnl.gov>, and follow

the directions onscreen. If you have any  
questions about the new IM process or if  
you need assistance with your document  
reviews, call the IM help line at  
ext. 2-IM4U (2-4648).

CMS wants to thank  
everyone who attended the  
author and reviewer training  
sessions in August. The IM  
team greatly appreciated your  
comments and feedback and has  
been working to implement some  
of your suggested improvements into the  
new system. ■



## CMS Scientist Briefs Secretary Tom Ridge on Radiation Detection for Homeland Security

On July 23, CMS scientist **Dan Archer** helped demonstrate Laboratory-developed radiation detection technologies to **Tom Ridge**, the secretary of the Department of Homeland Security. In the demonstration, Dan asked Secretary Ridge to carry a briefcase past an adaptable radiation area monitor (ARAM), which immediately indicated the presence of radioactive material and identified the quantity and type.

As the leader of the cross-directorate team that developed ARAM, Dan felt extremely honored that ARAM was chosen as one of the technologies to be shown to Secretary Ridge. Dan was also impressed by Secretary Ridge's ability to quickly grasp the various radiation detection technologies and assess their value to our nation.

ARAM, a portable, general-purpose monitor that Dan fondly calls "everyman's detector," can be used to screen

almost anything—people, packages, vehicles on the road—for radioactivity. ARAM's purposefully nondescript exterior cloaks a highly versatile device that instantly alerts its operator if it detects any type of radioactive material. For example, ARAM could be used at a border crossing to screen trucks without requiring them to stop. Trucks flagged by ARAM could then be investigated more thoroughly with additional radiation detection devices. Using ARAM in this way would safeguard our nation's security without impeding the flow of international commerce.

Dan, a Chemical Biology and Nuclear Science Division nuclear physicist matrixed to the Nonproliferation, Arms Control, and International Security Directorate, began working on ARAM with his team in mid-2002 and first demonstrated an ARAM prototype in December 2002 at an event



CMS scientist Dan Archer (right) with Tom Ridge (left), the secretary of the Department of Homeland Security, in front of the purposefully nondescript adaptable radiation area monitor (ARAM).

introducing Livermore's Homeland Security Organization. The Laboratory is currently in the process of licensing ARAM and is working with an industrial partner so that the instrument can be mass-produced and distributed to interested parties, such as government agencies, airports, and package couriers. ■

## \$5.9 Million Grant Awarded to a CNSAMR-Initiated Collaborative for a New NMR Spectrometer



An example of the three-story-high, 900-MHz NMR spectrometer to be installed at UC Berkeley.

The National Institutes of Health (NIH) recently awarded a \$5.9 million, five-year grant to a multi-institutional collaborative initiated by scientists in the Center for National Security Applications of Magnetic Resonance (CNSAMR), a joint effort between CMS

and the Biology and Biotechnology Research Program (BBRP) Directorate.

The grant, which was announced in early July, will enable the collaborative to procure and install a powerful 900-MHz (21.1-T) nuclear magnetic resonance (NMR) spectrometer for the Central California region. The magnetic field generated by the new spectrometer will be at least 200,000 times stronger than the magnetic field of Earth.

CNSAMR researchers (**Robert Maxwell** from CMS and **Monique Cosman** and **Krish Krishnan** from BBRP) spearheaded the grant

application process in August 2002 by inviting representatives from UC Berkeley, UC San Francisco, UC Santa Cruz, UC Davis, Stanford University, and Genentech to a CMS-funded planning meeting at the Wente Vineyards Restaurant in Livermore. The attendees selected a principal investigator (**David Wemmer** of UC Berkeley) and outlined their submission to NIH. They also decided to house the proposed spectrometer, which will weigh several tons and will stand three stories high, in UC Berkeley's Stanley Biosciences and Bioengineering Facility, a new building that is scheduled for completion in 2006.

In the NMR technique, researchers use magnetic fields to probe the structure and dynamics of molecules and materials, such as high-molecular-weight proteins, RNA, membrane proteins, and DNA-protein complexes. For example, NMR enables structural biologists

to study biological molecules in solution—their natural environment. NMR can also provide dynamic insight into the structural changes that occur as a protein folds and unfolds while carrying out its function.

By employing the unprecedented power of the new spectrometer's ultrahigh magnetic field, Livermore researchers expect to greatly expand their ongoing research efforts. In particular, CNSAMR scientists will be able to deepen their investigations of the proteins and biomolecular complexes that play important roles in cancer and other diseases, such as multiple sclerosis. ■



CNSAMR researchers (left to right): Krish Krishnan, Monique Cosman, and Robert Maxwell.

## Notable Publications BY MICHAEL FLUSS

### Unlocking the Mysteries of Protein Folding Kinetics

We all try to keep in shape, but protein molecules are the yoga champions of the nanoworld. Proteins are long chains of amino acids that can loop about, or fold, in many ways. However, each protein must fold in a specific way to function properly. Misfolded proteins can cause problems and have been linked to many diseases, such as Alzheimer's, cystic fibrosis, and cancer.

Protein folding kinetics can now be studied on the single-molecule level under nonequilibrium conditions, thanks to the development of a microfluidic mixer, as described in "Single-molecule measurement of protein folding kinetics" (*Science* **301**, 1233 [2003]), a notable publication coauthored by CMS's Lawrence Fellow **Olgica Bakajin**.

The new mixer enabled Olgica and her collaborators to monitor Förster resonance energy transfer after triggering a folding reaction in the cold shock protein. This information

helped them understand the sequence of events through which the protein changed from a random coil to its functional folded form. By using the mixer to study additional proteins, future researchers will be able to devise general rules for protein folding, leading to a better understanding of diseases caused by misfolded proteins and, eventually, better treatments.

#### Publication URL

<http://www.sciencemag.org/cgi/reprint/301/5637/1233.pdf> ■



CMS's Lawrence Fellow Olgica Bakajin

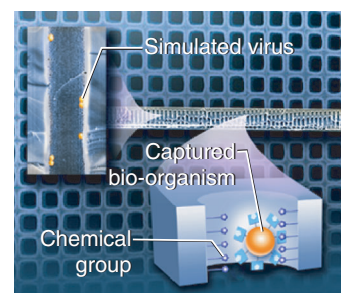
### Using Functionalized Silicon Membranes to Selectively Capture Bio-organisms

The Crusaders searched for the Holy Grail, but Laboratory researchers are searching for a "holey" grail—a new application of nanoscience in the area of biology.

The immobilization and detection of specific bio-organisms remain great technical challenges in many biomedical applications, including the decontamination or analysis of air and liquids (e.g., drinking water and body fluids). Achieving these goals will require the fabrication of materials with controlled pore diameter, length, and surface chemistry.

In the notable publication, "Functionalized silicon membranes for selective bio-organism capture" (*Nat. Mater.* **2**, 391 [2003]), CMS researchers **Sonia Létant**, **Bradley Hart**, **Tony Van Buuren**, and **Lou Terminello** described the first functionalized silicon (Si) membranes and demonstrated their ability to selectively capture simulated bio-organisms. The successful fabrication of these membranes opens the door to a new

Background: A scanning electron microscope (SEM) image showing the top view of a functionalized silicon (Si) membrane with 2- $\mu$ m pores. Top left: An enlarged SEM image of the cross section of a functionalized pore with 200-nm simulated viruses captured on the pore walls. Bottom right: A schematic of a captured bio-organism in a functionalized Si pore with the chemical groups that were attached during the functionalization process.



class of materials that are able to recognize the external fingerprints of bio-organisms—such as size and outer membrane proteins—for specific capture-and-detection applications.

#### Publication URL

<http://www.nature.com/cgi-taf/DynaPage.taf?file=/nmat/journal/v2/n6/full/nmat888.html&filetype=pdf> ■

### Phonon Dispersion Curves: A New Frontier in Plutonium Research

There certainly is "a whole lot of shaking going on"—in plutonium (Pu), that is! Recently, the first-ever experimentally determined phonon dispersion curves (PDCs) of a Pu alloy were reported in a notable publication, "Phonon dispersions of fcc  $\delta$ -plutonium-gallium by inelastic x-ray scattering" (*Science* **301**, 1078 [2003]), by CMS scientist **Joe Wong** and his colleagues ([see the Corner on Science article on p. 1](#)).

A microscopic picture of Pu PDCs had been considered unattainable because of the extreme experimental difficulties associated with inelastic neutron scattering, the standard method for measuring PDCs. However our researchers circumvented these difficulties by using the best third-generation synchrotron available, seizing on a new technique called high-resolution inelastic x-ray scattering, and exploiting it to the full.

This approach opens new experimental opportunities for future actinide research requiring single-crystal specimens,

especially for small and/or complex multiphase systems. The results of Wong et al.'s work show several unusual features, including a profound elastic anisotropy; an exceptionally small, shear elastic modulus  $C'$ ; a Kohn-like anomaly in the T1[011] branch; and a pronounced softening of the [111] transverse modes. These features can be related to the phase transformations of Pu and to the strong coupling between the lattice structure and the 5f valence instabilities. These results also provide a critical test for theoretical treatments of highly correlated 5f electron systems, as exemplified by recent many-body dynamical-mean-field-theory calculations for  $\delta$ -Pu by Dai et al. (*Science* **300**, 953 [2003]).

#### Publication URL

<http://www.sciencemag.org/cgi/reprint/301/5636/1078.pdf>

#### For more information

Visit the CMS Web site ([http://www-cms.llnl.gov/s-t/phonon\\_disp.html](http://www-cms.llnl.gov/s-t/phonon_disp.html)). ■

## Spotlight on Laboratory Directed Research and Development— Sparking Scientific Breakthroughs in CMS

The Laboratory Directed Research and Development (LDRD) Program invests funds in innovative science and engineering projects that ensure the scientific and technical vitality of the Laboratory and that enhance the Laboratory's ability to meet the challenges of its evolving missions.

LDRD projects are divided into four categories: (1) Strategic Initiatives, which set new directions for existing programs and/or develop new programmatic areas; (2) Exploratory Research studies, which

are aligned with the strategic R&D needs of a directorate or institute; (3) Laboratory-Wide projects, which allow researchers to propose research concepts with limited management filtering; and (4) Feasibility Study/Project Definition proposals, which provide researchers with the flexibility to explore the feasibility of new ideas.

CMS is proud that our scientists have developed many successful LDRD proposals because this work helps keep our scientists at the frontiers of their disciplines while strategically positioning our directorate for future technical

challenges. This is especially important for our younger scientists, both as a recruiting tool and as an opportunity that provides many valuable experiences in preparation for leadership roles in Laboratory programs.

Beginning with this issue of the CMS newsletter, we will be profiling new LDRD researchers in CMS—highlighting their cutting-edge research efforts and the role that LDRD played in helping them become part of our CMS community. ■

### New Contributor in LDRD: Julie Perkins

Julie Perkins was originally hired to work on an existing LDRD project, but the principal investigator's (PI's) subsequent departure from the Laboratory resulted in another job opportunity for Julie, who became the new PI for "Development of synthetic high-affinity ligands," an Exploratory Research in the Directorates project cosponsored by CMS and the Biology and Biotechnology Research Program Directorate.

Julie grew up in the United Kingdom, where she received her bachelor's degree in chemistry from Liverpool University in 1996 and her Ph.D. in chemistry from Sheffield University in 1999. While working as a postdoc at UCLA, Julie learned about the LDRD project's goal to create synthetic high-affinity ligands (SHALs), that is, ligands that bind to proteins with high affinity and specificity. Such SHALs have important potential applications for treating cancer and countering biowarfare.

The project fit well with Julie's background in synthetic chemistry. In addition, she was intrigued by the Laboratory's reputation as "a funky mix of academia and industry." Julie didn't want to be a pure academic, and she feared that a position in industry would quickly become repetitive and

mundane. She decided to accept the Laboratory's job offer and join the team of researchers at CMS's BioSecurity and Nanosciences Laboratory.

Since coming to Livermore in July 2001, Julie has focused on synthesizing SHALs that bind to tetanus toxin; botulinum toxin; and HLA-DR10, a protein expressed on the surface of non-Hodgkin's lymphoma. In collaboration with researchers both at Livermore and at the UC Davis Cancer Center, Julie synthesized a SHAL that binds to HLA-DR10. She also added a metal-chelating functionality to the SHAL. If all goes well, the SHAL will deliver the radioactive isotope yttrium-90 specifically to HLA-DR10 pro-

teins throughout a patient's body and in turn deliver radiation to the radiation-sensitive lymphoma.

Julie's first LDRD project ended in fiscal year 2003, and she has applied for additional LDRD funding to develop ligands for biological molecules by using dynamic combinatorial chemistry to increase the speed of specific ligand development. Looking back, Julie is amazed at the wealth of knowledge she has acquired about chemistry, biology, and oncology; bioconjugate and synthesis techniques; and laboratory instruments. Julie relishes the unpredictable nature of her work in CMS and looks forward to the new challenges ahead. ■



LDRD researcher Julie Perkins (right) and her summer student, Carlos Valdez (left), demonstrating the use of a semiautomatic synthesizer (top) and high-performance liquid chromatography (bottom).

## Postdoc News



### 2003 CMS Postdoctoral Symposium a Great Success!

The 2003 CMS Postdoctoral Symposium took place on July 16 in Building 235. The symposium, which featured more than 35 oral and poster presentations by CMS postdoctoral researchers, was an excellent display of the breadth and quality of research being conducted by our postdoctoral staff. To view some of the posters and presentations, visit [http://www-cms.llnl.gov/PostDocs/symp\\_7-03/presentations.html](http://www-cms.llnl.gov/PostDocs/symp_7-03/presentations.html).

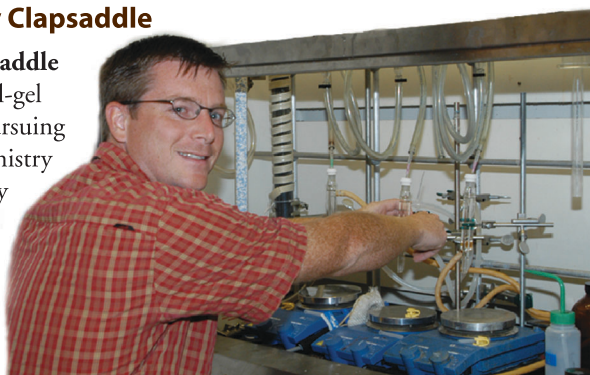
At the symposium, awards were presented to CMS postdocs **Kerri Blobaum** and **Sergei Kucheyev** (see p. 9). We thank all who attended the 2003 symposium and look forward to celebrating the research accomplishments of our CMS postdocs at next year's symposium. (To see more pictures from the symposium, visit [http://www-cms.llnl.gov/PostDocs/symp\\_7-03](http://www-cms.llnl.gov/PostDocs/symp_7-03).) ■

### Postdoc Profile: Brady Clapsaddle

CMS postdoc **Brady Clapsaddle** first entered the realm of sol-gel chemistry research while pursuing his Ph.D. in inorganic chemistry at Colorado State University (CSU). However, he did not fully appreciate the versatility within the field until after his arrival at the Laboratory in February 2002, when he greatly expanded his efforts in sol-gel chemistry.

As a member of the Advanced Material Synthesis Group working with **Joe Satcher** in the Chemistry and Chemical Engineering Division, Brady has been impressed by the many potential applications of sol-gel chemistry. For example, his current research projects use sol-gel chemistry to make novel materials (e.g., nanostructured energetic composites) as well as functionalized thin films for separation applications in matrix-assisted laser desorption/ionization (MALDI) mass spectrometry.

A high-school star athlete, Brady was recruited to play soccer at the University of St. Thomas in St. Paul, Minnesota. After graduating with a bachelor's degree in chemistry, he worked as a technician at 3M for a few years. Brady then entered graduate school, where he became friends with **Alex Gash**, a fellow Ph.D. student who



CMS postdoc Brady Clapsaddle setting up a synthetic reaction in a fume hood.

later joined CMS and helped bring Brady to the Laboratory. Brady's combined experience in industry and academia makes him particularly appreciative of the Laboratory's special culture, which lets him pursue both basic and applied research.

Brady is excited about his research efforts in sol-gel chemistry, which he views as a core methodology that can be used to explore many areas of science. For example, after presenting his research at the 2003 CMS Postdoctoral Symposium, Brady was approached by several CMS scientists, who suggested that he investigate using sol-gel materials in other fields, such as the preparation of carbon nanotubes and ceramics. Brady looks forward to further developing his expertise with sol-gel chemistry so that he can join other Livermore scientists in supporting projects across the Laboratory. ■



CMS Director's Review Committee chair Tom Tombrello (back row, furthest left) and CMS Associate Director Tomás Díaz de la Rubia (back row, second from the left) with some of the many postdocs, staff, and visitors who helped make the 2003 CMS Postdoctoral Symposium a successful event.

## Facilities/Operations News

### Volunteers Needed for the 2003 Run for HOME

CMS is hosting this year's Run for HOME, which will be held on Wednesday, October 29. Volunteers from all of CMS are needed to make sure that the run successfully kicks off the Laboratory's 2003 Helping Others More Effectively (HOME) Campaign.

The HOME Campaign offers Laboratory employees an opportunity each year to come together and assist those in need. The Run for HOME serves as a fun way to generate excitement about the HOME Campaign by encouraging people to attend the Agency Fair and learn firsthand about the nonprofit agencies featured in the HOME Campaign booklet.

The theme of this year's race is Team America—three cheers for the red, white, and blue. All participants are encouraged to dress up in theme-related costumes. Prizes will be given for individual and team costumes

in various categories, including CMS's special costume category: American heroes and patriotic icons.

CMS volunteers are needed to help with the following committees: entertainment; security, emergency services, and labor; food; agency greeters/setup; theme/costume awards/judges; and time scoring. Volunteers are asked to be available for the day of the run; specific time commitments vary by committee. All volunteers will receive a special appreciation gift consisting of a HOME Campaign hat, T-shirt, and button.

To volunteer at the 2003 Run for HOME, visit <http://cmsonly.llnl.gov/HOME/run-volunteer.html>, and fill out the online form. For additional information about volunteering at the race,



All volunteers for the 2003 Run for HOME will receive a HOME Campaign hat, T-shirt, and button.

contact **Kim Hallock** (ext. 3-3564). For general information about the 2003 Run for HOME, contact **Al Moser** (ext. 3-0326), the chair of the Run for HOME committee, or **Jana Marden** (ext. 2-6091), the principal assistant to the chair. ■

### AHJ-Required Inventory Ensures Safe Use of CMS Electrical Equipment



As part of the Laboratory's Authority Having Jurisdiction (AHJ) Electrical Program, CMS is conducting a room-by-room inventory of all

CMS electrical equipment. **Wayne Luedtka**, an AHJ-trained field representative, will check whether each piece of equipment has been certified by a nationally recognized testing laboratory (NRTL). Approved electrical equipment will receive a green AHJ label indicating that the equipment can be plugged into the Laboratory's power grid. Any uncertified equipment will be recorded in a database so that a plan can be developed to inspect and repair this equipment in the future.

The purpose of the AHJ-Electrical Program is to determine whether electrical equipment is safe for use. Equipment that has been certified by an NRTL is automatically approved for use at the Laboratory. All other types of electrical equipment must be inspected by an AHJ field rep before being connected to the Laboratory's power grid. See the AHJ Web site at [http://www-r.llnl.gov/es\\_and\\_h/ahj/](http://www-r.llnl.gov/es_and_h/ahj/) for specific exemptions and additional information about the AHJ-Electrical Program.

To have your electrical equipment inspected right away, call Wayne at ext. 3-1259 or **Rich Green** at ext. 2-5359. If you have any questions about the CMS AHJ-Electrical Program, please contact **Carey Bailey** at ext. 2-1295. ■

### Ergonomic Evaluations Put CMS Employees at Ease

Since the launch of the CMS Ergonomic Evaluation Program in July, a team of Hazards Control safety professionals has been visiting CMS employees and conducting brief interviews to prescreen them for potential ergonomic problems. If full ergonomic evaluations are needed, team members then schedule these evaluations for employees.

The program's goal is to ensure that every person who works for CMS or in a CMS space has the opportunity for an ergonomic evaluation.



With this in mind, team members are dropping by every office, laboratory, and workspace that is in a CMS-owned building or that is occupied by a CMS employee.

To set up an initial ergonomic assessment, call **Yolanda Villa** at ext. 3-2913. Otherwise, keep an eye out for your friendly safety professional, and take a little time out of your day when he or she visits to make sure that your workplace environment is ergonomically sound! ■



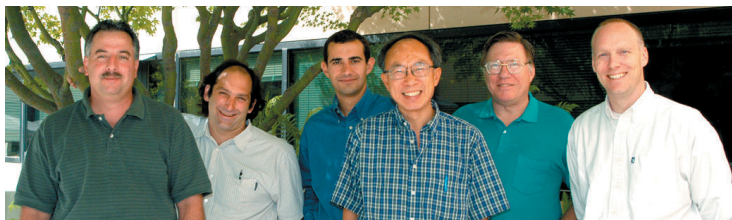
## Awards and Personnel News

### CMS-Led Team Receives the Laboratory's Top S&T Award

A team of scientists from the CMS and Energy & Environment (E&E) directorates has been awarded the Laboratory's Science and Technology Award by **Michael Anastasio**, director of the Laboratory. This award is the highest honor granted by the Laboratory for science and technology accomplishments.

**Joe Wong**, **Adam Schwartz**, and **Mark Wall** of CMS and **Dan Farber**, **Florent Occelli**, and **Carl Boro** of E&E received this award for their work measuring the phonon dispersion curves of  $\delta$ -plutonium–gallium. (See the [Corner on Science article on p. 1](#) and the [Notable Publications article on p. 4](#).)

According to **Tomás Díaz de la Rubia**, the CMS associate director, the team's efforts represent an outstanding example of world-class fundamental science inspired by the



The Laboratory's award-winning Pu phonon dispersion curve team (left to right): Mark Wall, Dan Farber, Florent Occelli, Joe Wong, Carl Boro, and Adam Schwartz.

mission-driven priorities of the Laboratory and of effective collaboration among a broad group of researchers.

CMS is proud to have cosponsored the team's groundbreaking research and looks forward to celebrating their accomplishments at the upcoming award ceremony with Director Anastasio. Congratulations to all team members! ■

#### Corner on Science

[Continued from page 1](#)

technique called high-resolution inelastic x-ray scattering (HRIXS). HRIXS uses x-rays rather than neutrons, thereby avoiding Pu's neutron absorption problem. Moreover, small sample size is not an issue with HRIXS because it can use the ultrabright x-ray beams of third-generation synchrotrons, such as the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, to analyze samples as small as  $10^{-4}$  mm<sup>3</sup>.

In February 2002, Joe traveled to ESRF and discussed his idea of using HRIXS to probe Pu phonons with **Michael Krisch**. Michael, a phonon research expert who developed and built a HRIXS beamline at ESRF for phonon dispersion measurements, was excited by Joe's idea, and they began a cross-Atlantic collaboration.

Joe then applied for Feasibility Study funding from the Laboratory Directed Research and Development (LDRD) Program. After receiving \$75,000 in March 2002, he worked with **Tai-C. Chiang's** research group at the University of Illinois, Urbana-Champaign. Their efforts at the Advanced Photon Source, a synchrotron facility at Argonne National Laboratory, demonstrated the use of x-rays for imaging Pu phonons.

This success helped Joe win additional LDRD funding. In October 2002, Joe and his coinvestigators, **Dan Farber** from the Energy and Environment (E&E) Directorate and **Adam Schwartz** from CMS, received \$400,000 in Exploratory Research in the Directorates funding (cosponsored by CMS, E&E, and Defense and Nuclear Technologies) to run their HRIXS experiments at ESRF, the only facility with a beamline capable of measuring Pu's lattice vibration energy.

Setting up the ESRF experiment was extremely challenging. Joe had to fill out extensive paperwork to receive Laboratory authorization for the experiment; ESRF beamtime, a scarce resource under high demand; and approval from French authorities to ship his Pu samples to Grenoble. Finally, Joe and his team, which included E&E postdoc

**Florent Occelli**, traveled to Grenoble in February 2003 and began running their experiment. Their eight-day, around-the-clock effort successfully mapped the three longitudinal phonon branches in Pu, but they discovered that a new sample holder design was needed to map the remaining four transverse branches.

Fueled by their initial success and the knowledge that another group was attempting the same measurements at Argonne, Joe and his team returned to Livermore and immediately redesigned a new sample holder with help from E&E's **Carl Boro**. They also made new Pu samples (with assistance from **Mark Wall** in CMS), applied for authorization to ship the new samples to Grenoble, and requested additional beamtime at ESRF. Amazingly, within four weeks, Joe and his team were back at ESRF for another eight days of conducting measurements around the clock. This time, they mapped all four transverse branches and obtained the first full PDCs ever determined for any Pu-bearing material.

After completing a detailed lattice dynamical analysis of the phonon data, Joe and his collaborators wrote up their findings. Their paper was submitted to *Science* in May, accepted in July, and published in August. Joe's first venture into Pu research had struck gold—ending a 40-year quest to determine Pu PDCs, opening the door to a new class of experimental research with microscale specimens, and benefiting the entire materials science and actinide research community.

#### For more information...

See the [Notable Publications article about Pu research on p. 4](#), and visit the CMS Web site ([http://www-cms.llnl.gov/s-t/phonon\\_disp.html](http://www-cms.llnl.gov/s-t/phonon_disp.html)).

#### Related publication

Wong, J. et al. Phonon dispersions of fcc  $\delta$ -plutonium–gallium by inelastic x-ray scattering. *Science* **301**, 1078 (2003). Available at <http://www.sciencemag.org/cgi/reprint/301/5636/1078.pdf>. ■

## Congratulations to Our Outstanding CMS Postdocs in 2003!

At the 2003 CMS Postdoctoral Symposium, **Tom Arsenlis**, the director of the CMS Postdoctoral Program, presented the following postdocs with awards in honor of their exceptional scientific achievements:

### Best of Symposium Poster Award

**Kerri Blobaum**—for her poster, “Investigating the  $\delta/\alpha'$  martensitic phase transformation in Pu–Ga alloys,” at the 2003 CMS Postdoctoral Symposium.

### Hal C. Graboske Jr. Postdoctoral Award

**Sergei Kucheyev**—for the most outstanding research contribution by a CMS postdoctoral researcher during the past year. ■



## Introducing Our CMS New Hires... Welcome Aboard!



Top row (left to right): **Nir Goldman**, CChED postdoc; **Jason Holt**, CBND postdoc; **Jennifer Burch**, MSTD physicist; and **Michael Harland**, MSTD senior technologist.

Bottom row (left to right): **Szczepan Roszak**, CChED faculty scholar; **Lucile Dauffy**, CBND postdoc; and **Lydia Hunt**, MSTD chemist.

## Saying Good-Bye to Our Retirees

CMS thanks the following individuals for their service to the Laboratory and wishes them a happy retirement!

**Allen Friensehner** began his Laboratory career in October 1963 as an electronics technician in the Engineering Directorate. At the time of his retirement on June 27, he was a senior scientific associate in CMS. Allen held an associate's degree in electronics technology and had recently received a second associate's degree in computer science in 2002.

**Bob McKoon**, a CMS chemical engineer, retired on June 30, ending a Laboratory career that began in May 1978 in mechanical engineering. Bob had a bachelor's degree in chemical engineering.

**Maureen Tortorelli** first came to the Laboratory in September 1978 as a senior accounting assistant. She retired on June 3, finishing her career as a division administrator in CMS's Materials Science and Technology Division. ■

### Interview With...

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Although new to CMS, Kim has a long history at the Laboratory. After receiving her bachelor's degree in physics from the University of Illinois at Chicago, Kim came to Livermore in 1987 as a graduate student researcher in the Department of Applied Science at UC Davis. She conducted her dissertation research in the Laser Program and received her Ph.D. in applied science in 1994. She was a postdoc in DNT's A Division and later became a staff scientist in the High-Energy-Density Experimental Sciences Program, where she performed experiments on the Nova and Omega laser facilities to study hydrodynamic instabilities and turbulent mixing in fluids. In 1999, Kim joined B Division as a primary designer. During her last year in DNT, Kim also served as the scientific editor for the Laboratory's magazine, *Science & Technology Review*.

While in B Division, Kim developed an interest in materials science: understanding how solids respond to dynamic loading—in particular, the problem of material failure. In an effort to create better predictive models for the codes used by weapons designers, she began to explore basic science research on material properties. Specifically, Kim worked with experimentalists, theorists, and modelers to investigate the response of materials to extreme dynamic conditions, such as the high-pressure, high-strain-rate deformations created by shock waves. As Kim's interest in materials science grew, moving into MSTD seemed like the next logical step of her Laboratory career.

In addition to her scientific responsibilities, Kim serves as an advocate for diversity in the technical workplace. She has visited other laboratories as a consultant to assess the workplace climate for technical women and believes that having women and minorities represented at all levels of management and decision making is critical to an organization's success. Kim actively recruits and supports younger women in science, and she is part of an ad hoc group that seeks to improve the climate for women in science. The group, which has organized several forums to discuss issues facing women in the technical workplace, assists senior management at the Laboratory in resolving these issues and encourages the building of support networks among Laboratory women.

Kim is excited to work with the many postdocs and researchers in CMS who are at the forefront of science. She plans to increase the participation of MSTD staff in dynamic experiments, particularly on novel, emerging platforms such as high-energy-density lasers (e.g., the National Ignition Facility [NIF]), and third- and fourth-generation light sources, so that the growing materials dynamics community can benefit from the extensive materials science expertise in MSTD. Finally, Kim intends to highlight and promote MSTD's many strengths so that the division's contributions to Laboratory programs, such as NIF and DNT, are evident to all. ■

**Message from the Associate Director**  
*Continued from page 1*

I also shared with you the importance of operations activities to our collective success and reaffirmed my commitment to safety, security, and financial integrity.

After a little more than a year in this job, I am in awe of our directorate's excellence and range of contributions. We are central to the Laboratory's present and critical to its future success. While I cannot mention every accomplishment, I would like to share a few highlights from the past fiscal year.

### Programmatic Accomplishments

Our scientists are an integral part of the NIF interdisciplinary team that has produced tremendous accomplishments during the past few years, and their efforts continue to improve the performance of NIF optics and other critical materials and components. At the same time, CMS scientists are helping define the science and technology (S&T) that will enable the development and efficient use of 2 $\omega$  light on NIF, as well as the development of optical components for the NIF High-Energy Petawatt Initiative.

CMS materials scientists are working closely with NIF and DNT physicists to design and execute high-power laser experiments to measure materials strength at high pressure. Our materials scientists and chemists have also teamed with Engineering, NIF, and DNT staff to explore long-range target-fabrication research and development (R&D) for future experiments on NIF.

Working with DNT, our directorate continues to meet all campaign milestones, including those in surveillance, enhanced surveillance, high explosives, and advanced simulation and computing. The final design for the new Energetic Materials Processing Center at Site 300 is underway, and we expect to break ground by 2005. In addition, our scientists have made outstanding contributions to stockpile stewardship, both by providing research insight into the aging of weapons components and by making sure that National Nuclear

Security Administration officials and government advisory panels understand the key issues regarding weapons aging.

Our presence in NAI is strong. CMS scientists have accepted important assignments both in Livermore and in Washington. They have also worked hard to help organize the new Department of Homeland Security.

We are well positioned to help the Laboratory execute any new projects in nuclear and radiation countermeasures, as well as chemical and biological nonproliferation and countermeasures. Scientists in the Glenn T. Seaborg Institute continue to develop novel gamma-ray imaging detectors for homeland security applications, while scientists in the Chemical Biology and Nuclear Science Division (CBND) have become critical players in nuclear forensics and attribution. The expertise and capabilities of our forensic scientists have been invoked on numerous occasions with tremendous success.

In E&E, CMS continues to play a central role in the Yucca Mountain Program (YMP). Our scientists have brought additional resources to the Laboratory from the Defense Advanced Research Projects Agency (DARPA) and from the Department of Energy's (DOE's) Civilian Radioactive Waste Program. The new work being funded is synergistic with the existing YMP mission and will help us define and execute ways to develop even more robust materials for nuclear waste isolation.

### The Laboratory's S&T Plan

Underlying all of these programmatic accomplishments is a strong base of fundamental S&T. Our management is actively involved in the crafting of the Laboratory's long-range S&T Plan. The

goal is to develop a vision of compelling, discovery-class science that will enhance existing programs and enable future missions. Six investment areas have been identified: high-energy-density science; stockpile stewardship R&D; science at the intersection of chemistry, materials, and biology; radiation, nuclear, and isotope science; information, simulation, and systems; and E&E. Our directorate contributes to all six areas and is central to both stockpile stewardship R&D and science at the intersection of chemistry, materials, and biology.

Working with DNT, Engineering, and the Physics and Applied Technologies Directorate, we have provided a road map for stockpile stewardship R&D investments headlined by the new Nanoscale Synthesis and Characterization Laboratory. In this plan, plutonium (Pu) science, extreme dynamics, and extreme chemistry round out a scientific agenda that will enable the achievement of stockpile stewardship goals far into the future.

The road map for science at the intersection of chemistry, materials, and biology, a joint effort with Engineering, the Biology and Biotechnology Research Program Directorate, and NAI/Homeland Security, is equally exciting. For example, one aspect of the plan focuses on identifying the nanoscience and nanotechnology challenges that are posed by expected future requirements for chemical and biological sensing.

### CMS's Organizing Themes

Within CMS, we have defined a set of four organizing themes that are highly synergistic with the Laboratory's investment areas. The following themes take advantage of our strengths and will guide our future strategic investments:

- Materials properties and performance under extreme conditions (MPPXC)
- Extreme chemistry and chemical engineering
- Science at the intersection of chemistry, materials, and biology



CMS scientists (Jerry Britten, front row, furthest left; Jim Peterson, front row, third from the left; and Curly Hoaglan, back row, second from the left) are part of the NIF petawatt team.

- Applied nuclear science for national-security and human-health applications

To better focus on these strategic areas, we have realigned our divisions: the Materials Science and Technology Division with MPPXC, the Chemistry and Chemical Engineering Division with extreme chemistry and chemical engineering, and CBND with the third and fourth themes. Articles will be published on the CMS Web site to describe the details of each organizing theme.

### Scientific Breakthroughs

CMS scientists have made outstanding contributions in fundamental science that is aligned with the mission-driven priorities of the Laboratory:

The BioSecurity and Nanosciences Laboratory (BSNL) continues to be a beacon of excellence. Every BSNL visitor is amazed at the creative energy that emanates from Building 154. In addition, our cadre of young chemists and materials scientists is doing an outstanding job of generating the type of award-winning science that is published in journals such as *Science*, the *Journal of the American Chemical Society*, and *Physical Review Letters*.

Significant new resources have been provided by agencies such as DARPA, the DOE Office of Nonproliferation Research and Engineering, and the Department of Defense for work on important topics like bioaerosol mass spectrometry and bioforensics. The Laboratory has also committed to the Pathomics Project—the quest for presymptomatic detection of infectious diseases—and CMS scientists are a vital and critical part of this effort.

With the same nuclear forensics capabilities used in international security, **Ian Hutcheon** and his team investigated isotope ratios in interplanetary media. This work enabled their definitive statements in a *Science* publication regarding the age of our solar system.

As discussed elsewhere in this newsletter, CMS scientists and their collaborators continue to make progress toward developing a deep and thorough understanding of Pu, our favorite metal.

### Safety and Operations Kudos

As I mentioned in *Newsline* earlier this year, simultaneous excellence in science and operations is a core value of the Laboratory. The professionalism and dedication of our operations staff are superb. Our safety record is excellent, and I want to thank all of you—scientists, engineers, technicians, operations staff, everyone—for your commitment and dedication to our core value.

Remember, our goal is zero injuries. Please don't forget to take two seconds to think before beginning a routine operation, two minutes to review your work plan for the day and your integration work sheet (IWS), and two hours to go over a new activity and IWS.

Our Information Systems team protected us from many computer worms and pests. The team's outstanding work was recognized in a national magazine.

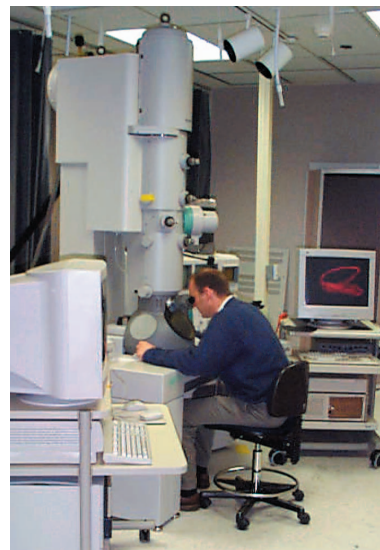
We met Laboratory goals by successfully finding and tagging 99.8% of our property and equipment. Our teams renovated and refurbished laboratories now used for the Bioaerosol Laboratory, the Center for National Security Applications of Magnetic Resonance, and the NanoSIMS Laboratory.

We inaugurated Building 155 and completed the seismic retrofit of Building 151. Thanks for all of your patience and sacrifice during this necessary retrofit. Your dedication has ensured the safe housing of CMS employees.

### Looking Ahead to FY04

As you can see, FY03 was an amazing year filled with tremendous accomplishments. I appreciate all of your dedication and hard work. And now let's look forward to an exciting FY04:

CMS scientists will continue to be a central part of the effort to build out and fully use NIF. Our staff will help make and install optics faster, better, and cheaper. We will also help ensure that the ambitious schedule for line replaceable units stays on target. In addition, we will play critical roles in assuring cleanliness during operations, maintaining high production rates for continuous phase plates, making disposable debris



CMS scientist Adam Schwartz using a transmission electron microscope to study the effects of plutonium aging.

shields, and increasing the robustness of the production process for large crystals.

We will conduct important work on the W80 Life Extension Program, the budget line item for the Energetic Materials Center, and the deployment of stockpile surveillance tools to ensure the safety and integrity of our country's nuclear deterrent. CMS staff will also be key collaborators on the first NIF experiments for stockpile stewardship.

We will continue to play a crucial role in NAI and in the new Livermore effort in support of homeland security. A CMS staff member in Washington, D.C., will manage the nuclear radiation part of the Homeland Security investment portfolio, and another CMS staff member will lead the multinational laboratory effort to provide cargo security to the New York/New Jersey Port Authority.

In E&E, CMS scientists will provide leadership to the YMP licensing application and S&T program.

Finally, we will have new equipment, including a dynamic transmission electron microscope, a focused ion beam, a fast diamond anvil cell, and equipment with new synthesis capabilities.

It will be a great year!

Cheers,  
Tomás ■

## Conference Calendar

DATE	CONFERENCE	LOCATION	WEB SITE
October 5–10, 2003	Ninth Frontiers of Electron Microscopy in Materials Science Conference	Berkeley, CA	<a href="http://femms2003.llnl.gov">http://femms2003.llnl.gov</a>
November 2–5, 2003	Seventh International Symposium on Aerogels	Alexandria, VA	<a href="http://www.sainc.com/isa7">http://www.sainc.com/isa7</a>
November 16–20, 2003	Second International Conference of the Chemistry and Physics of the Transactinide Elements	Napa, CA	<a href="http://tan03.lbl.gov">http://tan03.lbl.gov</a>
December 1–5, 2003	2003 Materials Research Society Fall Meeting	Boston, MA	<a href="http://www.mrs.org/meetings/fall2003">http://www.mrs.org/meetings/fall2003</a>

### Ninth Frontiers of Electron Microscopy in Materials Science Conference

The Frontiers of Electron Microscopy in Materials Science (FEMMS) conference is a biennial meeting focused on the application of electron microscopy. **Wayne King**, a scientist in the Materials Science and Technology Division (MSTD), has been a primary organizer of FEMMS since its early years.

The Laboratory continues to be a major sponsor of this conference, and this year's organizing committee includes Wayne, several of his MSTD colleagues (**Geoffrey Campbell**, **Alex Hamza**, **Mukul Kumar**, **Kevin Moore**, **Bryan Reed**, **Adam Schwartz**, **Mark Wall**, and **Alexander Ziegler**), and CMS Chief Technologist **David Eaglesham**.

### Seventh International Symposium on Aerogels

All aspects of aerogels and other ultraporous nanoarchitectures will be discussed at the Seventh International Symposium on Aerogels.

Two scientists in the Chemistry and Chemical Engineering Division (CChED), **Ted Baumann** and **Alex Gash**, will deliver keynote speeches. Ted will describe the "Synthesis of metal-doped organic and carbon aerogels," while Alex will discuss "Metal oxide aerogels using organic epoxides: Synthesis, characterization, and applications."

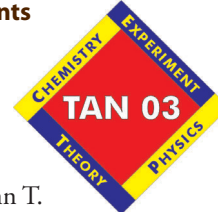
Additional talks will be given by **John Reynolds**, a scientist in the Chemical Biology and Nuclear Science Division (CBND), and CChED scientists **Brady Clapsaddle** and **Tom Tillotson**. In addition, CChED scientist **John Poco** will present a poster on "Aerogel production capabilities at LLNL."

**FEMMS 2003**

### Second International Conference of the Chemistry and Physics of the Transactinide Elements

A wide spectrum of nuclear chemistry and physics related to the transactinides will be covered at the Second International Conference of the Chemistry and Physics of the Transactinide Elements (TAN 03).

TAN 03 is cosponsored by CMS's Glenn T. Seaborg Institute, and CBND scientist **Ken Moody** is a conference cochair. The TAN 03 organizing committee also includes CBND scientists **Joshua Patin**, **Dawn Shaughnessy**, **Mark Stoyer**, and **John Wild**.



### 2003 Materials Research Society Fall Meeting

The Fall 2003 meeting of the Materials Research Society will feature two symposia organized by CMS scientists.

**Randy Simpson**, the CChED division leader, is co-organizing a symposium called "Synthesis, characterization, and properties of energetic/reactive nanomaterials," while MSTD scientist **Jim Tobin** is organizing a four-day symposium, "Actinides: Basic science, applications, and technology." ■



Please send items for the next newsletter (e.g., directorate news, awards, conference calendar items) to **Emmeline Chen** ([chen8@llnl.gov](mailto:chen8@llnl.gov)).

A PDF of this newsletter with clickable Web links can be downloaded from the CMS Web site: <http://www-cms.llnl.gov/news/newsletter.html>.